ISCR

Institute for Scientific Computing Research

Fiscal Year 2000 Annual Report

http://www.llnl.gov/casc/iscr/

Lawrence Livermore National Laboratory
P.O. Box 808, L-561, Livermore, CA 94551

CASC

Center for Applied Scientific Computing

UNIVERSITY RELATIONS PROGRAM

The University Relations Program (URP) encourages collaborative research between Lawrence Livermore National Laboratory (LLNL) and the University of California campuses. The Institute for Scientific Computing Research (ISCR) actively participates in such collaborative research, and this report details the Fiscal Year 2000 projects jointly served by URP and ISCR. For a full discussion of all URP projects in FY 2000, please request a copy of the URP FY 2000 Annual Report by contacting

Lawrence Livermore National Laboratory
Christina M. Budwine, University Relations Program
P. O. Box 808, L-413
Livermore, CA 94551

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Contents

The Mission of the ISCR

The Institute for Scientific Computing Research (ISCR) at Lawrence Livermore National Laboratory is jointly administered by the Center for Applied Scientific Computing (CASC) and the University Relations Program (URP), and this joint relationship expresses its mission. An extensively externally networked ISCR cost-effectively expands the level and scope of national computational science expertise available to the laboratory through CASC. The URP, with its infrastructure for managing five institutes and numerous educational programs at LLNL, assumes much of the logistical burden that is unavoidable in bridging the laboratory's internal computational research environment with that of the academic community.

As large-scale simulations on the parallel platforms of DOE's Accelerated Strategic Computing Initiative become increasingly important to the overall mission of LLNL, the role of the ISCR expands in importance, accordingly.

Relying primarily on non-permanent staffing, the ISCR complements laboratory research in areas of the computer and information sciences that are needed at the frontier of laboratory missions. The ISCR strives to be the "eyes and ears" of the laboratory in the computer and information sciences, in keeping the laboratory aware of and connected to important external advances. It also attempts to be "feet and hands," in carrying those advances into the laboratory and incorporating them into practice. In addition to conducting research, the ISCR provides continuing education opportunities to laboratory personnel, in the form of on-site workshops taught by experts on novel software or hardware technologies.

The ISCR also seeks to influence the research community external to the laboratory to pursue laboratory-related interests and to train the workforce that will be required by the laboratory. Part of the performance of this function is interpreting to the external community appropriate (unclassified) aspects of the laboratory's own contributions to the computer and information sciences—contributions that its unique mission and unique resources give it a unique opportunity and responsibility to make.

Of the three principal means of packaging scientific ideas for transfer—people, papers, and software—experience suggests that the most effective means is people. The programs of the ISCR are therefore people-intensive.

Finally, the ISCR, together with CASC, confers an organizational identity on the burgeoning computer and information sciences research activity at LLNL and serves as a point of contact within the laboratory for computer and information scientists from outside.

Institute for Scientific Computing Research
Fiscal Year 2000 Director's Report

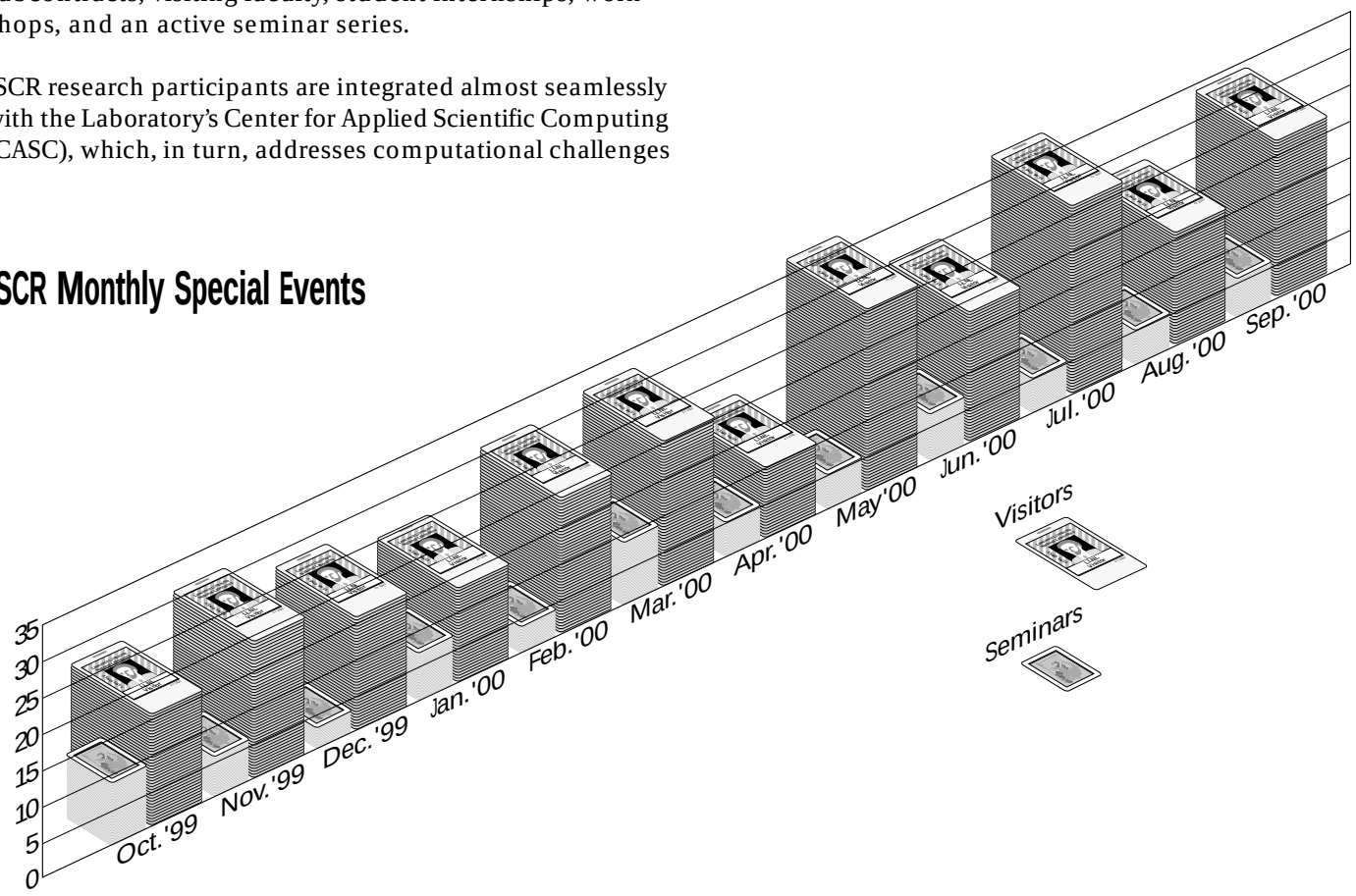
Large-scale scientific computation, and all of the disciplines that support it and help to validate it, have been placed at the focus of Lawrence Livermore National Laboratory by the Accelerated Strategic Computing Initiative. The Laboratory operates the computer with the highest peak performance in the world and has undertaken some of the largest and most compute-intensive simulations ever performed. However, computers at architectural extremes are notoriously difficult to use efficiently, and successes (such as the Laboratory's two Bell Prizes awarded in November 1999) only point out the need for much better ways of interacting with the results of large-scale simulations.

Advances in scientific computing research have therefore never been more vital to the core missions of the Laboratory than at present. Computational science is evolving so rapidly along every one of its research fronts that to remain on the leading edge, the Laboratory must engage researchers at many academic centers of excellence. In FY 2000, the Institute for Scientific Computing Research (ISCR) has expanded the Laboratory's bridge to the academic community in the form of collaborative subcontracts, visiting faculty, student internships, workshops, and an active seminar series.

ISCR research participants are integrated almost seamlessly with the Laboratory's Center for Applied Scientific Computing (CASC), which, in turn, addresses computational challenges arising throughout the Laboratory. Administratively, the ISCR flourishes under the Laboratory's University Relations Program (URP). Together with the other four Institutes of the URP, it navigates a course that allows the Laboratory to benefit from academic exchanges while preserving national security. While FY 2000 brought more than its share of challenges to the operation of an academic-like research enterprise within the context of a national security laboratory, the results declare the challenges well met and worth the continued effort.

Fiscal year 2000 was the first full year under Acting Director David Keyes. Keyes, the Richard F. Barry Chair of Mathematics & Statistics at Old Dominion University and an ISCR faculty participant since October 1997, dedicated half of his time to the technical program of the ISCR. Jill Dunaway continued as the full-time Institute Administrator. Leslie Bills continued her support on the seminar series and Terry Garrigan came aboard in time to help with the very large summer program and program expansions in other areas, as indicated below.

ISCR Monthly Special Events



In FY 2000, we launched our ASCI Institute for Terascale Simulation Lecture Series, featuring visits from Fred Brooks, Peter Lax, Burton Smith, and Gilbert Strang. A special section of this annual report is devoted to the abstracts and biosketches of these distinguished lecturers. The ITS Lectures typically draw two to three hundred people from around the laboratory and surrounding scientific community. They are archived on video and available at the LLNL Technical Library. We plan to continue this series with approximately six "movers and shakers" in high-end simulation and its enabling technologies per year.

In April, the ISCR co-sponsored the annual *Copper Mountain Conference*, in Copper Mountain Colorado. The 2000 meeting was devoted to Iterative Methods. Eight members of the CASC scientific staff presented papers, as did twenty of the academic collaborators of the ISCR.

In May, the ISCR organized a three-day *Power Programming Short Course* to enable laboratory code developers (in CASC and in the other divisions) to come to grips, in advance, with the ASCI White machine, of which the laboratory took delivery late in the year. The instructors were Steve White of IBM, Larry Carter of UCSD, David Culler of UCB, Clint Whalley of the University of Tennessee, and Bill Gropp of Argonne. Sixty-five people attended.

In June, with the advent of our large student summer program and sponsorship from the Defense Programs office of DOE HQ, we launched an *Internships in Terascale Simulation Technology* tutorial series, a ten-week series with two-lectures per week. The tutors included three of LLNL's recent computational science textbook authors (Alice Koniges, John May, and Van Henson), five LLNL computational physicists (David Brown, Garry Rodrigue, Howard Scott, Alek Shestakov, and Lin Yang), CASC computer scientist Gary Kumfert, and the ISCR Director. Koniges' *Industrial-Strength Scientific Computing* and May's *Parallel I/O* were published by Morgan-Kaufman during FY 2000. Henson co-authored, with Bill Briggs and Steve McCormick, a recent update of Briggs' "best selling" 1987 monograph, *A Multigrid Tutorial*. Though intended for students, permanent CASC researchers attended an occasional subseries of the lectures.

In July, under the direction of CASC scientist Carol Woodward, the ISCR organized a three-day *Workshop on Solution Methods for Large-scale Nonlinear Problems* at a hotel in nearby Pleasanton. This workshop was capped at 48 attendees, for good discussions. This workshop was an ASCI-context successor to a 1995 workshop with a similar title organized by Professor Homer Walker (now Chair of Mathematical Sciences at WPI). Also dubbed, *The Rootfinders' Ball*, the attendance list of this workshop reads like a "Who's Who" in parallel implicit methods for PDEs. A special issue of Linear Algebra and its Applications with papers drawn from the workshop is being guest-edited by organizer Woodward and CASC colleague Panayot Vassilevski.

We also in July co-sponsored a two-day *Workshop on Mining Scientific Data Sets*. Professor Vipin Kumar, an ASCI Level-2 collaborator, was the host at the Army HPC Research Center at the University of Minnesota, and CASC scientist Chandrika Kamath was a co-organizer. Livermore affiliates provided three of the talks. Most of the principals in the nascent field of scientific data mining were among the 110 in attendance.

Rounding out the very busy month of July, the ISCR co-hosted the *Computational Science Graduate Fellows Conference*, providing local organization and a substantial part of the technical program for this three-day conference. The Krell Institute, which manages the CSGF program for the Department of Energy, made the most of this immersive technical get-together, bringing 38 of their fellows to join the 7 who were already interning at CASC in the ISCR summer student program.

Completing the year's technical meetings, the ISCR co-sponsored the *Fifth Symposium on Overset Grids and Solution Technology* at UC Davis. CASC scientist David Brown was a co-organizer. Six members of CASC and three ISCR affiliates presented work carried out in the laboratory's OVERTURE and SAMRAI frameworks.

In FY 2000, the ISCR brought to the laboratory a vigorous contingent of post-docs, faculty visitors, and students. Twenty faculty visitors were in residence for more than just a seminar visit—for a week to a semester. Eight post-docs made the ISCR their home this past year. We also had 55 students in residence, mostly for 8–10 weeks of the summer, but several of them for a semester or a full year. Each of these students was in a research relationship with one of CASC's 87 full-time technical staff.

Looking ahead, the ISCR anticipates co-sponsorship of post-docs with the new NSF Institute for Pure and Applied Mathematics (IPAM) at UCLA. IPAM co-directors Mark Green, Eitan Tadmor, and Tony Chan consider LLNL's ISCR to be a prime off-campus partner.

The pages of this report summarize the activities of the faculty members, post-doctoral researchers, students, and guests from industry and other laboratories who participated in LLNL's computational mission under the auspices of the ISCR during FY 2000. Altogether, the ISCR hosted 220 visits from 158 different visitors, who gave a total of 72 seminars on site. The vast majority of the visitors were from academia, with 11% from industry and 13% from other laboratories. Visitors from outside of the United States made up 6% of the total. The histograms on page 4 chart the numbers of visitors and seminars as a function of the month of the fiscal year.

Most of the material of this annual report comes directly from the visitors and principal investigators of the projects being reported, who selected formats convenient for their purposes. We thank Dan Moore and Linda Moore of the Technical Information Division of LLNL for their graphic artistry in producing an easily navigated and visually pleasing document.

We hope that you enjoy examining this report on the ISCR's diverse activities in FY 2000. For further information about the Institute, please contact us at the address below. Inquiries about how you might enhance the on-going FY 2001 program at the ISCR, or beyond, are welcome.

David Keyes

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ISCR Fiscal Year 2000 in Review

FY 2000 Seminar Series (in reverse chronological order)

Gabriel Wittum, University of Heidelberg ..... September 29, 2000
Klaus Stueben, GMD—Forschungszentrum Informationstechnik GmbH ..... September 28, 2000
Luis Chacon, Los Alamos National Laboratory ..... September 27, 2000
Alfred Inselberg, San Diego Supercomputer Center ..... September 22, 2000
Marty Itzkowitz, Sun Microsystems, Inc. ..... September 15, 2000
Sutanu Sarkar, University of California, San Diego ..... September 13, 2000
Gundolf Haase, Johannes Kepler University, Linz ..... September 11, 2000
Paul Reynolds, University of Virginia ..... August 28, 2000
Ed Seidel, Max-Planck-Institut fuer Graviationsphysik ..... August 25, 2000
Ariel Shamir, University of Texas, Austin ..... August 10, 2000
Gregory Balls, University of California, Berkeley ..... August 9, 2000
Randy Bank, University of California, San Diego ..... August 8, 2000
Michael Holst, University of California, San Diego ..... August 1, 2000
Beth Anne Bennett, Yale University ..... July 25, 2000
Zhiqiang Cai, Purdue University ..... July 24, 2000
Steven Allmaras, Boeing ..... July 19, 2000
Gregory Forest, University of North Carolina ..... June 27, 2000
Saul Abarbanel, Tel Aviv University ..... June 14, 2000
Craig Douglas, University of Kentucky ..... June 12, 2000
Barton Miller, University of Wisconsin ..... June 12, 2000
Sean Peisert, San Diego Supercomputer Center ..... June 8, 2000
Kenneth Powell, University of Michigan ..... June 5, 2000
Stephan Knapek, University of Bonn ..... May 31, 2000
Anthony Skjellum, MPI Software Technologies, Inc. ..... May 25, 2000
Eitan Tadmor, University of California, Los Angeles ..... May 18, 2000
Eitan Tadmor, University of California, Los Angeles ..... May 18, 2000
Iain Duff, CCLRC Rutherford Appleton Laboratory ..... May 9, 2000
Karl Warnick, University of Illinois, Urbana-Champaign ..... April 28, 2000
Gerhard Zumbusch, University of Bonn ..... April 25, 2000
X. Sherry Li, Lawrence Berkeley Laboratory ..... April 13, 2000
Padhriac Smyth, University of California, Irvine ..... April 6, 2000
Omar Ghattas, Carnegie Mellon University ..... March 29, 2000
Jan Hesthaven, Brown University ..... March 28, 2000
Jan Hesthaven, Brown University ..... March 27, 2000
Rob Van Der Wijngaart, MRJ Technology Solutions, NASA Ames Research Center ..... March 24, 2000
Joel Saltz, University of Maryland ..... March 23, 2000
N. Radhakrishnan and Raju Namburu, U.S. Army Research Laboratory (ARL) ..... March 16, 2000
Eric DeSturler, University of Illinois, Urbana-Champaign ..... March 14, 2000
Gil Chita, TakeFive Software ..... March 13, 2000

FY 2000 Seminar Series (in reverse chronological order) continued:

Luiz De Rose, IBM TJ Watson Research Center ..... March 7, 2000
Harvey Wasserman, Los Alamos National Laboratory ..... March 3, 2000
Dimitri Mavriplis, ICASE NASA Langley Research Center ..... March 2, 2000
Inez Heinz, Lawrence Livermore National Laboratory ..... February 28, 2000
Gabriel Wittum, University of Heidelberg ..... February 24, 2000
Gerald Hedstrom, LLNL Retiree ..... February 23, 2000
David Padua, University of Illinois ..... February 11, 2000
Hanan Samet, University of Maryland, College Park ..... January 28, 2000
John Quagliano, Los Alamos National Laboratory ..... January 27, 2000
John Quagliano, Los Alamos National Laboratory ..... January 27, 2000
Allen Malony, University of Oregon ..... January 24, 2000
Steve Chapin, Syracuse University ..... January 19, 2000
Alok Choudhary, Northwestern University ..... January 14, 2000
Petter Bjorstad, University of Bergen, Norway ..... January 13, 2000
Art Mirin, Lawrence Livermore National Laboratory ..... January 11, 2000
Linda Stals, Old Dominion University ..... January 6, 2000
Jong Kim, Pohang University of Science and Technology ..... December 14, 1999
Michael Donaldson, Merant ..... December 13, 1999
Sally McKee, University of Utah ..... December 13, 1999
Garth Gibson, Carnegie Mellon University ..... December 2, 1999
V. Ralph Algazi, University of California, Davis ..... November 23, 1999
Jeremy Siek, University of Notre Dame ..... November 22, 1999
Andrew Lumsdaine, University of Notre Dame ..... November 22, 1999
Peter Vanderbilt, MRJ Technology Solutions ..... November 12, 1999
Jeff Hollingworth, University of Maryland, College Park ..... November 2, 1999
Pat Miller, Scientific Computing Applications Division ..... October 20, 1999
Michael Burl, Jet Propulsion Laboratory ..... October 18, 1999
Roy Hemker, University of California, Los Angeles ..... October 15, 1999
Dean Dauger, University of California, Los Angeles ..... October 7, 1999
David Young, The Boeing Company ..... October 5, 1999
Timothy Kelley, North Carolina State University ..... October 4, 1999

FY 2000 Institute for Terascale Simulation Lecture Series

Frederick P. Brooks, University of North Carolina ..... August 30, 2000
Peter Lax, Courant Institute of the Mathematical Sciences, New York University ..... June 9, 2000
Burton Smith, Tera Computer Company ..... May 12, 2000
Gilbert Strang, Massachusetts Institute of Technology ..... April 12, 2000

Visiting Faculty, Guests, Consultants, and Researchers

Visiting and Collaborating Professors

Xiao-Chuan Cai, University of Colorado
David Dean, Front Range Scientific Computations, Inc.
Jack Dongarra, University of Tennessee
Craig Douglas, University of Kentucky
Alejandro Garcia, San Jose State University
Michael Griebel, University of California, San Diego
Nicholas Hadjiconstantinou, Massachusetts Institute of Technology
Michael Holst, University of California, San Diego
Kenneth Joy, University of California, Davis
Karen Karavanic, Portland State University
David Keyes, Old Dominion University
Raytcho Lazarov, Texas A&M University
Byung Lee, University of Vermont
Dimitri Mavriplis, ICASE, NASA Langley Research Center
James McWilliams, University of California, Los Angeles
Christoph Pflaum, University of Wurzburg
Calvin Ribbens, Virginia Polytechnic Institute and State University
John Ruge, Front Range Scientific Computations, Inc.
Donald Schwendeman, Rensselaer Polytechnic Institute
Padhraic Smyth, University of California, Irvine
Robert Snapp, University of Vermont

Participating Guests

Mark Adams, University of California, Berkeley
Marsha Berger, New York University
William Bosl, Stanford University
Marian Brezina, University of Colorado
George Byrne, Illinois Institute of Technology
Roger Crawfis, Ohio State University
David Dean, University of Colorado
Eric de Sturler, University of Illinois
John Fitzgerald, Lawrence Livermore National Laboratory (retired)
Kyle Gallivan, Florida State University
Michael Gertz, University of California, Davis
Michael Griebel, University of Bonn
Bernd Hamann, University of California, Davis
Ulf Hannebutte, Intel Corporation
Stanley Johnson, Lehigh University

Participating Guests (continued)

Kenneth Joy, University of California, Davis
Johannes Kraus, University of Leoben
Raytcho Lazarov, Texas A&M University
Andrea Malagoli, University of Chicago
Michael Minion, University of North Carolina
Joseph Pasciak, Texas A&M University
Michael Pernice, University of Utah
Elbridge Gerry Puckett, University of California, Davis
John Rice, University of California, Berkeley
Ulrich Ruede, University of Erlangen
Thomas Rutaganira, American River College
Yousef Saad, University of Minnesota
Paul Saylor, University of Illinois
Daniel Schikore, Computational Engineering, International
Rob Van Der Wijngaart, NASA Ames Research Center
Gabriel Wittum, University of Heidelberg
Daniel Wolitzer, California State University, Hayward
Ytha Yu, California State University, Hayward
Ludmil Zikatanov, Pennsylvania State University
Gerhard Zumbusch, University of Bonn

Consultants

Bernie Alder, University of California (Professor Emeritus)
Randolph Bank, University of California, San Diego
Leo Breiman, University of California, Berkeley
Harry Dwyer, University of California, Davis
Anne Greenbaum, University of Washington
Chuck Hansen, University of Utah
David Keyes, Old Dominion University
Heinz-Otto Kreiss, University of California, Los Angeles
Thomas Manteuffel, University of Colorado
Stephen McCormick, University of Colorado
Linda Petzold, University of California, Santa Barbara
Steve Schaffer, New Mexico Tech
Homer Walker, Worcester Polytechnic Institute

Department of Applied Science Faculty

Nelson Max
Garry Rodrigue

Postdoctoral Researchers

Robert Anderson
Erick Cantu-Paz
Petri Fast
Jean-Luc Fattebert
Raymond Fellers
Imola Fodor
Barry Lee
Luc Machiels
Brian Miller
Thomas Rutaganira
Leonid Tsap

University Collaborative Research Program Subcontractors

Scott Baden, University of California, San Diego
Jackson Beatty, University of California, Los Angeles
John Dawson, University of California, Los Angeles
Jeffrey Gregg, University of California, Davis
B. S. Manjunath, University of California, Santa Barbara
Warren Mori, University of California, Los Angeles
Linda Petzold, University of California, Santa Barbara
Joachim Raeder, University of California, Los Angeles
Andrew Szeri, University of California, Berkeley

LDRD Project Investigators

Mark Duchaineau, LLNL, Center for Applied Scientific Computing
Chandrika Kamath, LLNL, Center for Applied Scientific Computing

Students

Student Guests

Nathan Crane, University of Illinois
Matt Giamporcaro, Boston University
Charles Hindman, University of Colorado
Jason Hunt, University of Michigan
McKay Hyde, California Institute of Technology
David Hysom, Old Dominion University
Lars Karlsson, Chalmers University of Technology

Student Guests (continued)

Falko Kuester, University of California, Davis
Diem Phuong Nguyen, University of Utah
Stefan Nilsson, Chalmers Institute of Technology
Christopher Oehmen, University of Tennessee
Wing Yee, University of Utah

Department of Applied Science Students

Paul Covello
Rebecca Darlington
Ana Iontcheva
Joseph Koning
Daniel Laney
Sean Lehman
Tim Pierce
Jonathan Rochez
Subhasis Saha
Bahrad Sokhansanj
Jay Thomas
Michael Wickett

ISCR Students

Marcel Arndt, University of Bonn
Travis Austin, University of Colorado
Zachary Belanger, Oakland University
Martin Bertram, University of California, Davis
Melvina Blackgoat, Northern Arizona University
Kathleen Bonnell, University of California, Davis
Timothy Chartier, University of Colorado
Tom Dossa, Santa Clara University
Jochen Garcke, University of Bonn
Aaron Herrnstein, University of California, Davis
Chisup Kim, Texas A&M University
Imelda Kirby, University of Washington
Stephan Knapek, University of Bonn
Frank Koster, University of Bonn
David Nault, University of Cincinnati

ISCR Students (continued)

Serban Porumbescu, University of California, Davis
Robert Rieben, University of California, Davis
M. Alex Schweitzer, University of Bonn
Danny Thorne, University of Kentucky
Stanimire Tomov, Texas A&M University
Clinton Torres, Northern Arizona University
Serge van Criekingen, Northwestern University
Kevin Vlack, University of Illinois

ITST Students

Lucas Ackerman, Worcester Polytechnic Institute
Brian Ball, Worcester Polytechnic Institute
Janine Bennett, University of California, Davis
Richard Cook, University of California, Davis
Michael Flanagan, Texas A&M University
David Hysom, Old Dominion University
Linh Lieu, University of California, Davis
David Littau, University of Minnesota
Michael McCracken, Penn State University
Jason Morgan, University of Utah
Joshua Senecal, University of California, Davis

National Physical Science Consortium (NPSC) Students

Rachel Karchin, University of California, Santa Cruz
Imelda Kirby, University of Washington
Megan Thomas, University of California, Berkeley

Workshops and Conferences

Common Component Architecture (CCA) Forum, Oakland, CA, March 2000
Copper Mountain Conference, Copper Mountain, CO, April 2000
Power Programming Short Course, Livermore, CA, May 2000
Workshop on Mining Scientific Datasets, Minneapolis, MN, July 2000
Solution Methods for Large-Scale Nonlinear Problems, Pleasanton, CA, July 2000
CSGF Conference, Livermore, CA, July 2000
5th Symposium on Overset Grids & Solution Technology, Davis, CA, September 2000